Bose-Einstein Condensates in optical lattices: study of its experimental signatures

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DECLARATION

I hereby declare that the work which is being presented in the thesis entitled Bose-Einstein Condensates in optical lattices in partial fulfillment of the requirement for the award of the degree of Master of Science, submitted in the Department of Physics and Astronomy, National Institute of Technology Rourkela is an authentic record of the reproduced results done by me under the supervision of Prof. Sanjoy Datta. The matter embodied in this thesis has not been submitted in other institution or university for the award of any other degree or diploma.

Jayash Panigrahi

This is to certify that the above statement made by the candidate is correct to the best of my knowledge.

Prof. Sanjoy Datta
July, 2015

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1. INTRODUCTION

1.1 ***The Ultracold atoms***

The realization of Bose-Einstein Condensation(BEC) in ultracold dilute atomic gases in 1995 opened up new avenues for studying many quantum phenomenons on a microscopic scale. In these experiments one can simulate the microscopic Hamiltonian of the condensed matter system in much detail and can have precise control over the various parameters of the system. One can study the spectroscopic and coherent properties of the experimental system in exceptional detail. This is exciting, because various properties of solid state systems can be studied using ultracold atoms in an optical lattice as it provides much more precise experimental control over conventional experiments and is configurable for different paradigms. Innumerable experiments in this field have been performed. Atomic species such as Rubidium, Sodium, Potassium, Cesium, Ytterbium, Lithium, Hydrogen, metastable Helium and Chromium have been used to produce Bose Einstein Condensates (BECs). To obtain temperatures on a scale of few microKelvin(required for BEC), these experiments use a combination of laser cooling and evaporative cooling techniques [1][2] [4]). The BECs in cold atomic gases, produced in experiments are weakly interacting. It can be used to study their coherence and superfluid properties and can also be used for broader range of applications, especially in recreating and probing condensed matter physics. Recently, these cold systems have played vital role in the experimental study of entanglement and quantum information processing and more importantly in the realization of qubits(a quantum analogue of Bit)[5].

1.2 ***Optical lattices***

Artificial lattices can be created by applying laser light in three dimensions in such a way that it produces standing waves, thus a periodic potential, into which one can load cold gases. The physics of interacting bosons in its simplest form can be described by Bose-Hubbard lattice models. This model can be modified according to different spin and lattice configurations as per the research interest in condensed mater physics. Which means the Hamiltonian can be simulated in the experiments with wide range of control over many relevant parameters involved with the system. By using various combination of lattice parameters and external fields, it is possible to control the dynamics involved with atoms in an optical lattices [7]. From previous experiments, we can see that the interaction energies in a system can be controlled by altering the lattice depth, deeper lattice depth implies lower tunneling rates within the lattice sites, effectively leading to stronger interactions among the atoms. Similarly, by manipulating the polarization of the laser involved, one can produce spin dependent(for same atomic species with two different internal state) optical lattice can be produced [8].

Of most of the systems in condensed matter physics, optical lattices provide better isolation from the environment, which is an important factor in studying coherent properties on a longer timescale. An immediate application of BECs in optical lattices is to use it as a quantum simulator,to simulate various lattice models.

1.3 Outline

In this thesis, we make an attempt to study the Bose-Einstein Condensations in an optical lattice. After the introduction of BECs and optical lattices in Chap. 2, in the next chapter the Bose-Hubbard Model is presented for a fixed number of particles. In Chap. 3, the Hamiltonian for our system of fixed particles is solved by applying Hatree Fock Bogoliubov Popov formalism and the condensate density is calculated.

2. BACKGROUND: BEC AND OPTICAL LATTICES

Since the first experimental creation of Bose Einstein Condensates(BEC) in dilute gases, there have been an incredible proliferation of different quantum systems in which BEC's have been achieved. Various atomic species have been condensed such as $^{87}Rb,^{23}Na,^{1}H,^{85}Rb,^{4}He$ [2] and more recently ^{164}Dy and ^{168}Ev [6]. Early condensates were created using magneto-optical traps which provided an axially symmetric, harmonic potential [7] and condensates in lattices geometry can also be created by applying an optical lattice [3][6] .

2.1 *Bose-Einstein Condensate*

According to Bose Einstein Distribution for a bosonic particle, decrease in temperature causes increase in number of particles in the ground state. The occupation number of the ground state N_0 becomes comparable to total number of atoms N in the system. The state of such macrocscopic occupation is called Bose-Einstein condensation, where a macroscopic matter wave forms when the wave packet of atoms starts to overlapping with each other. The de Broglie wavelength of such an atom is $\lambda_{dB} = \sqrt{2\pi\hbar^2/mk_BT}$, and the atomic distance is $n^{1/3}$ (n = density). For the formation of a macroscopic matter wave the condition is

$$\lambda_{dB} \sim n^{1/3} \tag{2.1}$$

The Bose-Einstein Distribution is given by

$$n\,(E) = \frac{1}{e^{E/K_BT} - 1} \tag{2.2}$$

Since the particle number is conserved, a chemical potential introduced μ and total number is fixed such that,

$$N = \Sigma \frac{1}{e^{(\epsilon_k - \mu)/K_BT} - 1}, \epsilon_k = \frac{\hbar^2 k^2}{2m} \tag{2.3}$$

we know that $\Sigma_k \longrightarrow_{\Omega_d \to \infty} \int \frac{D^d k}{(2\pi)^d}$ is in 'd' dimensions, where Ω_d is the d-dimensional volume. For d=3 we have,

$$n = \frac{N}{\Omega_3} = \int \frac{D^3 k}{(2\pi)^3} \frac{1}{e^{(\epsilon_k - \mu)/K_BT} - 1} \tag{2.4}$$

$$= \int dk \frac{k^2}{(2\pi)^2} \frac{1}{e^{(\epsilon_k - \mu)/K_B T} - 1} \tag{2.5}$$

$$= \frac{1}{\hbar^3} \left\{ \frac{K_B T_m}{2\pi} \right\}^{3/2} Li_{3/2}(\frac{\mu}{K_B} T) \tag{2.6}$$

The condensate fraction N_0/N can be expressed as

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_0} \right)^{3/2} \tag{2.7}$$

which is a function of temperature. The temperature of the cold gas consists of two components, the one due to the condensates and due to thermal gases. The condensate wave function of a Bose-Einstein condensate is given by

$$\psi(r, t) = \sqrt{n(r, t)} e^{i\phi(r,t)} \tag{2.8}$$

where $n(r, t) = |\psi(r, t)|^2$ is the density of the condensate[3].

2.2 *Optical Lattices*

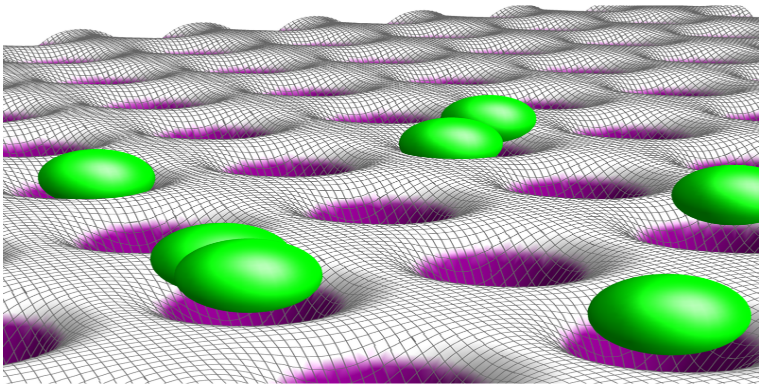

Fig. 2.1: Visualization of atoms in an optical lattice using equation 2.12. See appendix 6.2 for the Mathematica code

The interference of two laser beams with the same frequency and polarization propagating in opposite directions, leads to periodic pattern of intensity which also acts as a periodic potential for atoms. The interference between two laser beams leads to a total electric field $E(\overrightarrow{r}, t)$ and intensity $I(\overrightarrow{r}, t)$ [7].

$$\begin{aligned} E_{\overrightarrow{r},t} = & \quad E_1(\overrightarrow{r}, t) + E_2(\overrightarrow{r}, t) \\ = & \quad E_1 \widehat{e}_1 exp[i(\overrightarrow{k}_1 . \overrightarrow{r} - \omega_1 t)] + E_2 \widehat{e}_2 exp[i(\overrightarrow{k}_2 . \overrightarrow{r} - \omega_2 t)] \quad (2.9) \\ & \quad (2.10) \end{aligned}$$

Thus,

$$\begin{aligned} I(\overrightarrow{r},t) \propto &\quad E(\overrightarrow{r},t).E(\overrightarrow{r},t) \\ = &\quad E_1^2 + E_2^2 + 2(\hat{e}_1 - \hat{e}_2)Re[E_1 E_2^* e^{i(\overrightarrow{k}_1 - \overrightarrow{k}_2).\overrightarrow{r}(\omega_1-\omega_2)t)} \end{aligned} \quad (2.11)$$

From the interference pattern of two laser beams, we can infer that, the polarization product $\overrightarrow{e}_1.\overrightarrow{e}_2$ determines the optical lattice. The relative detuning $\Delta\omega \equiv \omega_1 - \omega_2$ can be described in three different cases [8]

1. $\Delta\omega = 0$, for a stationary optical lattice
2. for a moving lattice $\delta\omega \neq 0$
3. for a time averaged optical dipole trap where $\omega_{rec} \rightarrow$ recoil frequency,which is defined by $\hbar\omega_{rec} = \hbar^2 k^2/2m$

at $\Delta\omega = 0$ the interference term becomes a periodic potential given by $V \sim sin(\Delta k.r)$, when the two laser beams propagate in opposite direction, thus $\Delta k = 2k$ and $V \sim sin(2kz)$.

1. For such a optical lattice the period is given by $2\pi/2k = \lambda/2$, λ being the wavelength of a laser beam which can be controlled by changing the angle θ between the two beams. Thus, the resulting potential is $V \sim sin([2ksin(\theta/2)]x)$.
2. When $0 < \Delta\omega \sim \omega_{rec}$ the phase of the interference pattern becomes $\Delta kz - \Delta\omega t$ and the lattice moves with the speed $v = \Delta\omega/\Delta k$. For the case of counter-propagating beams ($k_1 = -k_2$), the speed now becomes $v = \Delta\omega/\Delta k = \Delta\omega/2k = \frac{\lambda}{2}\Delta f$, with $\Delta\omega = 2\pi\Delta f$
3. When $\omega_{rec} \ll \Delta\omega$ the interference pattern of two laser beams oscillation becomes fast compared the timescale of inter-atomic motion, thus the third term in the intensity relation (Eqn. 2.) gets averaged out to zero .

For our case we consider an optical lattice created by using similar frequency counter-propagating laser beams. The lattice potential becomes

$$V_{latt}(r,z) = -V_{latt} sin(2kz) \left\{ 1 - 2(\frac{r}{\omega_0})^2 - (\frac{z}{\omega_{z_R}})^2 \right\} \quad (2.12)$$

where ω_{z_R} is the Rayleigh length given by $\omega_{z_R} = \pi\omega_0^2/\lambda$ and ω_0 is beam waist of the laser used.

3. CONDENSATES IN OPTICAL LATTICES

3.1 Introduction

Ultracold atoms in optical lattices has been broadly used as a model for studying various condensed matter phenomenons. Ultracold atomic system in optical lattice is an ideal implementations of the Bose-Hubbard model and could serve as a quantum simulator to investigate condensed matter theories [8] [3]. This setup has major advantages over conventional condensed matter systems as

1. The system is defect-free.
2. The interaction is not as complicated as in conventional condensed matter system. The interaction is mainly due to s-wave collisions. (p-wave collisions could be implemented).
3. The experimental parameters can be controlled easily, precisely and dynamically. This is usually carried out by controlling the optical power of optical lattice laser beams.
4. Various optical lattice geometries can be implemented (i.e. simple cubic, triangular)

Quantum phase transition between the superfluid and Mott insulator phases for low-dimensional systems (1D) have already been achieved and studied with optical lattices. Various other theoretical proposal are awaiting to be experimentally realized using ultracold atoms and optical lattices [1] [2][6]. Currently experimental research groups are working towards the realization of ferro and anti-ferromagnetism, disordered systems , (Bose glass, Anderson localization), spinor system in optical lattice, quantum information processing, frustrated antiferromagnetism, dipolar gas system etc. [2].

We first study the BEC in non-interacting system and introduce the Bose Hubbard Model to study the BECs in an optical lattices. In the next chapter, we apply the Hartee Fock Bogoliubov method with Popov approximation(HFBP). This method allows us to calculate the properties of the condensates and the excitation properties. Then we study the theoretical signatures of the Bose-Einstein Condensates of an ultracold Bose gas on an homogeneous optical lattices at finite temperature. So at first we learn the formalism to solve the Hamiltonian of this system. In the following section we start with the Hamiltonian of the system and then transform it to the Bose- Hubbard Hamiltonian by expanding the Bose operators in the Wannier function [11][13]. Then we transform it to the momentum space by using creation and annihilation operators and apply the Bogoliubov approach, which consists of replacing the creation and annihilation operators by the total particles in condensate state plus the average fluctuations[13]. Then we diagonalize the effective Hamiltonian using Bogoliubov transformation and obtain the eigenvalues and hence the condensate density as well. This formalism in combined with local density approximation is applied to characterize a trapped BEC at finite temperature. The Hamiltonian for this system can be written as

$$\begin{aligned} H &= \int d^3(r)\Psi^\dagger(r)\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{latt}(r) + V_0(r)\right]\Psi(r) + \\ & \frac{U_b}{2}\int d^3(r)\Psi^\dagger(r)\Psi^\dagger(r)\Psi(r)\Psi(r) \end{aligned} \tag{3.1}$$

where the lattice potential $V_{latt} = V_0\sum_{i=x,y,z} Sin^2\frac{\pi r_i}{d}$ with 'd' the lattice spacing and V_0 is the lattice depth. The global harmonic trapping potential $V(x) = \frac{mw^2r^r}{2}$ and the s-wave interaction $U_b = \frac{4\pi\hbar^2 a_s}{m}$.

3.2 ***The Bose-Hubbard Model***

Here we study the finite temperature characteristics and the experimental signatures for a fixed total number of bosonic particles. In the recent studies, when the temperature is increased the system undergoes a phase transition from superfluid to normal state [13]. Were start with the basic many-body Hamiltonian to describe the system of interacting ultracold atoms inside an optical lattice. In the Hamiltonian given by eq (3.1), the field operator $\Psi(r)$ can be expanded in Wannier functions $w_n(r)$, since they are a complete basis set. The Wannier functions $w_n(r)$ get reduced to the ground band Wannier functions $w(r) = w_0(r)$ and the field operator $\Psi(r)$ can be written as $\Psi(r) = \sum_i w_0(r - R_i)a_i$, where a_i is the annihilation operator of the cold atoms with lattice site i with position R_i of the lattice [8][3]. Considering the three terms in the above Hamiltonian eq. (3.1).

1. The hopping matrix element t describes the hopping or tunneling between adjacent sites and is given by

$$-t\sum_{<i,j>} a_i^\dagger a_j \text{ with } t = \int drw^*(r - R_i)(-\frac{\hbar^2}{2m}\Delta^2 + V_{latt}(r))w(r - R_j) \tag{3.2}$$

where $< i, j >$ denote the nearest neighbor lattice sites. The hopping term has negative sign because the delocalization lowers the kinetic energy.

2. The trapping potential term gives an energy offset at each lattice site.

$$\sum_i \epsilon_i \hat{n}_i \text{ with } \epsilon_i = \int drw^*(r-R_i)V_{latt}(r)w(r-R_j) \rightarrow V_{latt}(R_i) \quad (3.3)$$

where n_i is the number operator given by $\hat{n}_i = a_i^\dagger a_i$

3. The last term describes the onsite interaction energy, which we consider as s-wave interaction and $U(r_1, r_2) = g\delta(r_1 - r_2)$ [19]. Thus we can re write as

$$\frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1) \text{ with } U = g\int dr|w(r)|^4 = \frac{4\pi\hbar^2 a_s}{m}\int dr|w(r)|^4 \quad (3.4)$$

With these terms and introducing the chemical potential we obtain the Bose Hubbard Hamiltonian as

$$H = -t\sum_{<i,j>} a_i^\dagger a_j + \frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1) + \sum_i(\epsilon_i - \mu)\hat{n}_i \quad (3.5)$$

Now describing each subsystem as a uniform Hamiltonian and introducing creation and annihilation operators $a_{\mathbf{k}}^\dagger$ and $a_{\mathbf{k}}$ to transform it into momentum space by

$$a_i = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} a_{\mathbf{k}} e^{-i\mathbf{k}.r_i} \text{ and } a_i^\dagger = \frac{1}{\sqrt{V}}\sum_k a_{\mathbf{k}}^\dagger e^{i\mathbf{k}.r_i} \quad (3.6)$$

where V is the dimensionless quantization volume, which is the number of lattice sites. Now, substituting the above transformation to the Bose Hubbard Hamiltonian, the hopping term becomes,

$$\begin{aligned}
&= -t\sum_{<i,j>} a_i^\dagger a_j \\
&= -\frac{t}{V}\sum_{i,\delta}\sum_{\mathbf{k},\mathbf{k}'} a_{\mathbf{k}}^\dagger e^{i\mathbf{k}.\mathbf{r}_i} a_{\mathbf{k}'} e^{-i\mathbf{k}.(\mathbf{r}_i+\delta)} \\
&= -\frac{t}{V}\sum_{\delta}\sum_{\mathbf{k},\mathbf{k}'} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}\left(\sum_i e^{-i(\mathbf{k}-\mathbf{k}').\mathbf{r}_i}\right) e^{-i\mathbf{k}'.\delta} \\
&= -\frac{t}{\cancel{V}}\sum_{\delta}\sum_{\mathbf{k},\mathbf{k}'} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\cancel{V}\delta(\mathbf{k}-\mathbf{k}')e^{i\mathbf{k}'\delta} \\
&= -t\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}\sum_{\delta} e^{-i\mathbf{k}'.\delta} \\
&= -2.t\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} Cos(\mathbf{k}.\delta) \quad (3.7)
\end{aligned}$$

$$= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a^{\dagger}_{\mathbf{k}} a_{\mathbf{k'}} \tag{3.8}$$

where $\epsilon_{\mathbf{k}} = -2tCos(\mathbf{k}\delta)$ and $|\delta| = 1$. Now for the potential energy term : $\frac{U}{2}\sum_i a^{\dagger}_i a^{\dagger}_i a_i a_i$, using the similar transformation.

$$\begin{aligned}
&= \frac{U}{2V} \sum_{i,\mathbf{k},\mathbf{k'},q} a^{\dagger}_{\mathbf{k}} e^{-i\mathbf{k}.\mathbf{r}_i} a^{\dagger}_{\mathbf{k}+q} e^{i(\mathbf{k}+\mathbf{q}).\mathbf{r}_i} a_{k'+q} e^{-i(\mathbf{k'}+\mathbf{q}).\mathbf{r}_i} a_{\mathbf{k'}} e^{-i(\mathbf{k'})} \\
&= \frac{U}{2V} \sum_{i,\mathbf{k},\mathbf{k'},q} a^{\dagger}_{\mathbf{k}} a^{\dagger}_{\mathbf{k}+q} e^{-i(\mathbf{k}-\mathbf{k'}).\mathbf{r}_i} a_{\mathbf{k'}+q} a_{\mathbf{k'}} e^{-i(-\mathbf{k'}+\mathbf{k}).r_i} \\
&= \frac{U}{2V} \sum_{\mathbf{k},\mathbf{k'},q} a^{\dagger}_{\mathbf{k}} a^{\dagger}_{\mathbf{k}+q} \left(\sum_i e^{-i(\mathbf{k}-\mathbf{k'}).\mathbf{r}_i}\right) a_{\mathbf{k'}+q} a_{\mathbf{k'}} \left(\sum_i e^{-i(-\mathbf{k'}+\mathbf{k}).r_i}\right) \\
&= \frac{U}{2V} \sum_{\mathbf{k},\mathbf{k'},q} a^{\dagger}_{\mathbf{k}} a^{\dagger}_{\mathbf{k}+q} \left(\delta(\mathbf{k}-\mathbf{k'})\right) a_{\mathbf{k'}+q} a_{\mathbf{k'}} \left(\delta(-\mathbf{k'}+\mathbf{k})\right)
\end{aligned} \tag{3.9}$$

replacing $k \to -k$ and $k' \to -k'$ we get,

$$\begin{aligned}
&= \frac{U}{2V} \sum_{\mathbf{k},\mathbf{k'},q} a^{\dagger}_{\mathbf{k}+q} a_{\mathbf{k'}+q} \delta(\mathbf{k}-\mathbf{k'}) a^{\dagger}_{-\mathbf{k}} a_{-\mathbf{k'}} \delta(\mathbf{k}-\mathbf{k'}) \\
&= \frac{U}{2V} \sum_{\mathbf{k},\mathbf{k'},q} a^{\dagger}_{\mathbf{k}+q} a_{\mathbf{k'}+q} a^{\dagger}_{-\mathbf{k}} a_{-\mathbf{k'}}
\end{aligned} \tag{3.10}$$

Since we are going to deal with the untrapped system first, we only retain the last term $-\sum_i \mu a^{\dagger}_i a_i$,

$$\begin{aligned}
&= \sum_i \mu a^{\dagger}_i a_i \\
&= -\frac{\mu}{V} \sum_i \sum_{\mathbf{k},\mathbf{k'}} a^{\dagger}_{\mathbf{k}} e^{i\mathbf{k}.\mathbf{r}_i} a_{\mathbf{k'}} e^{-i\mathbf{k'}.(\mathbf{r}_i)} \\
&= -\frac{\mu}{V} \sum_{\delta} \sum_{\mathbf{k},\mathbf{k'}} a^{\dagger}_{\mathbf{k}} a_{\mathbf{k'}} \left(\sum_i e^{-i(\mathbf{k}-\mathbf{k'}).\mathbf{r}_i}\right) \\
&= \frac{\mu}{\cancel{V}} \sum_{\mathbf{k},\mathbf{k'}} a^{\dagger}_{\mathbf{k}} a_{\mathbf{k}} \cancel{V} \delta(\mathbf{k}-\mathbf{k'}) = \mu \sum_{\mathbf{k}} a^{\dagger}_{\mathbf{k}} a_{\mathbf{k}}
\end{aligned} \tag{3.11}$$

putting together the obtained transformations for the three terms of the Bose Hubbard Hamiltonian as,

$$\frac{U}{2V} \sum_{\mathbf{k},\mathbf{k'},q} a^{\dagger}_{\mathbf{k}+q} a_{\mathbf{k'}+q} a^{\dagger}_{-\mathbf{k}} a_{-\mathbf{k'}} + \sum_{\mathbf{k},\mathbf{k'}} (\epsilon_{\mathbf{k}} - \mu)\, a^{\dagger}_{\mathbf{k}} a_{\mathbf{k}} \tag{3.12}$$

3.3 Hartee Fock Bogoliubov Popov (HFBP) formalism

We apply the Hartee Fock Bogoliubov Popov (HFBP) formalism and at first focus on obtaining the eigenvalue of to characterize the thermal transition and superfluid properties[9]. For a condensed Bose gas, the average number of atoms N_o is a number much larger than one, which means that $N_0 = \langle a_0^\dagger a_0 \rangle \approx \langle a_0 a_0^\dagger \rangle$ and we can take $N_0 = \langle a_0^\dagger \rangle \langle a_0 \rangle$. Since $\langle a_0^\dagger \rangle$ and $\langle a_0 \rangle$ are the hermitian conjugates of each other, so we conclude that $\langle a_0^\dagger \rangle = \langle a_0 \rangle = \sqrt{N_o}$ [13]. The Bogoliubov approach consists of replacing the creation and annihilation operators by the average fluctuation plus $\sqrt{N_o}$.

$$a_o^\dagger \to \sqrt{N_0} + a_o^\dagger \text{ and } a_o \to \sqrt{N_0} + a_o \tag{3.13}$$

minimizing the energy of the gas with respect to the condensates number N_o and retaining only the leading order contribution, the interaction part of the Hamiltonian can be simplified.

$$\frac{U}{2V} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \sum_{k''} \sum_{\mathbf{k}'''} a_k^\dagger a_{\mathbf{k}'} a_{-\mathbf{k}''}^\dagger a_{-\mathbf{k}'''} \delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''} + \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu)\, a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \tag{3.14}$$

where,

$$\delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''} = \left\{ \begin{matrix} 0 \text{ for } \mathbf{k}+\mathbf{k}' \neq \mathbf{k}''+\mathbf{k}''' \\ 1 \text{ for } \mathbf{k}+\mathbf{k}' = \mathbf{k}''+\mathbf{k}''' \end{matrix} \right\} \tag{3.15}$$

by conservation of momentum we have $\mathbf{k}''' = \mathbf{k} + \mathbf{k}' - \mathbf{k}''$ and obtaining the terms for all cases of $\delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''}$
for the case when $\mathbf{k} = \mathbf{k}' = \mathbf{0}, \mathbf{k}'' \neq 0$, we have

$$a_0^\dagger a_0 a_{\mathbf{k}''}^\dagger a_{-\mathbf{k}''} \tag{3.16}$$

for the case when $\mathbf{k}'' = \mathbf{k}' = \mathbf{0}, \mathbf{k} \neq 0$, we have

$$a_0^\dagger a_0 a_{\mathbf{k}''}^\dagger a_{-\mathbf{k}''} = a_0^\dagger a_0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \tag{3.17}$$

for the case when $\mathbf{k} = \mathbf{k}'' = \mathbf{0}, \mathbf{k}' \neq 0$, we have

$$a_0^\dagger a_{\mathbf{k}'} a_0^\dagger a_{\mathbf{k}'} = a_0^\dagger a_0 a_{\mathbf{k}'}^\dagger a_{\mathbf{k}'} \tag{3.18}$$

for the case when $\mathbf{k} = -\mathbf{k}', \mathbf{k}'' \neq 0$, we have

$$a_{-\mathbf{k}}^\dagger a_{\mathbf{k}}^\dagger a_0 a_0 \tag{3.19}$$

for the case when $\mathbf{k} = \mathbf{k}'', \mathbf{k}' \neq 0$, we have

$$a_{-\mathbf{k}}^\dagger a_0^\dagger a_{\mathbf{k}} a_0 \tag{3.20}$$

for the case when $\mathbf{k} = \mathbf{0}, \mathbf{k}' = \mathbf{k}'' \neq 0$, we have

$$a_0^\dagger a_{\mathbf{k}'}^\dagger a_{\mathbf{k}'} a_0 \tag{3.21}$$

and adding the 6 terms we get,

$$\sum_{\mathbf{k}} \left[a_0^\dagger a_0^\dagger a_{\mathbf{k}} a_{-\mathbf{k}} + 4 a_0^\dagger a_0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_0 a_0 a_{-\mathbf{k}}^\dagger a_{\mathbf{k}}^\dagger \right] \tag{3.22}$$

Now, replacing the creation and annihilation operators by the average fluctuation plus $\sqrt{N_o}$, as

$$a_0^\dagger \to \sqrt{N_o} + a_0^\dagger \text{ and } a_0 \to \sqrt{N_o} + a_0 \tag{3.23}$$

and collecting the quadratic terms we get,

$$\sum_{\mathbf{k}} \left[N_o a_{\mathbf{k}} a_{-\mathbf{k}} + 4 N_o a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + N_o a_{-\mathbf{k}}^\dagger a_{\mathbf{k}}^\dagger \right] \tag{3.24}$$

The effective Hamiltonian is given by,

$$H^{eff} = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{U n_0}{2} \sum_{\mathbf{k}} \left(a_{\mathbf{k}}^\dagger a_{-\mathbf{k}} + 4 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger a_{\mathbf{k}}^\dagger \right) \tag{3.25}$$

Simplifying a little more by applying the commutation relationship $[a_{\mathbf{k}}, a_{\mathbf{k}}^\dagger] = 1$, we get

$$\begin{aligned} H^{eff} &= -\frac{1}{2} U n_0 N_o - \frac{1}{2} \sum (\epsilon_{\mathbf{k}} - \mu) \\ &+ \frac{1}{2} \sum_{\mathbf{k}} \left(a_{\mathbf{k}}^\dagger, a_{-\mathbf{k}} \right) \times \begin{bmatrix} \epsilon_{\mathbf{k}} + U n_0 & U n_0 \\ U n_0 & \epsilon_{\mathbf{k}} + U n_0 \end{bmatrix} \begin{bmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^\dagger \end{bmatrix} \end{aligned} \tag{3.26}$$

Here the term $a_{\mathbf{k}}^\dagger$ and $a_{\mathbf{k}}$ commutes and generates extra zeroth order terms. To diagonalize the effective Hamiltonian, we use Bogoliubov transformation. The transformation is given by,

$$\begin{bmatrix} b_{\mathbf{k}} \\ b_{-\mathbf{k}}^\dagger \end{bmatrix} = \begin{bmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ v_{\mathbf{k}}^* & u_{\mathbf{k}}^* \end{bmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^\dagger \end{pmatrix} = \mathbf{B} \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^\dagger \end{pmatrix} \tag{3.27}$$

to get $a_{\mathbf{k}}$ and $a_{-\mathbf{k}}^\dagger$ in terms of $b_{-\mathbf{k}}^\dagger$ and $b_{\mathbf{k}}$, B^{-1} is multiplied both sides of the above matrix.

$$\begin{aligned} \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^\dagger \end{pmatrix} &= \begin{bmatrix} b_{\mathbf{k}} u_{\mathbf{k}}^* - v_{\mathbf{k}} b_{-\mathbf{k}}^\dagger / (u_{\mathbf{k}} u_{\mathbf{k}}^* - v_{\mathbf{k}} v_{\mathbf{k}}^*) \\ b_{-\mathbf{k}}^\dagger u_{\mathbf{k}} - v_{\mathbf{k}}^* b_{\mathbf{k}} / (u_{\mathbf{k}} u_{\mathbf{k}}^* - v_{\mathbf{k}} v_{\mathbf{k}}^*) \end{bmatrix} \\ &= \frac{1}{(\mid u \mid^2 - \mid v \mid^2)} \begin{bmatrix} b_k u_{\mathbf{k}}^* - v_{\mathbf{k}} b_{-\mathbf{k}}^\dagger \\ b_{-\mathbf{k}}^\dagger u_{\mathbf{k}} - v_{\mathbf{k}}^* b_{\mathbf{k}} \end{bmatrix} \end{aligned} \tag{3.28}$$

Now,by substituting it in Eqn. (3.26) we get (illustrating only the last terms),

$$\begin{aligned} &\frac{1}{(\mid u \mid^2 - \mid v \mid^2)^2} \left[b_{\mathbf{k}} u_{\mathbf{k}}^* - v_{\mathbf{k}} b_{-\mathbf{k}}^\dagger, b_{-\mathbf{k}}^\dagger u_{\mathbf{k}} - v_{\mathbf{k}}^* b_{\mathbf{k}} \right] \begin{bmatrix} \epsilon_{\mathbf{k}} + U n_0 & U n_0 \\ U n_0 & \epsilon_{\mathbf{k}} + U n_0 \end{bmatrix} \\ &\times \begin{bmatrix} b_{\mathbf{k}} u_{\mathbf{k}}^* - v_{\mathbf{k}} b_{-\mathbf{k}}^\dagger \\ b_{-\mathbf{k}}^\dagger u_{\mathbf{k}} - v_{\mathbf{k}}^* b_{\mathbf{k}} \end{bmatrix} \end{aligned} \tag{3.29}$$

As $b^{\dagger}_{\mathbf{k}}$ and $b_{\mathbf{k}}$ follows standard commutation relations applicable for creation and annihilation operators for bosons, the matrix **B** also follows,

$$|\, u_{\mathbf{k}} \,|^2 - |\, v_{\mathbf{k}} \,|^2 = 1 \tag{3.30}$$

Substituting $a_{\mathbf{k}}, a^{\dagger}_{-\mathbf{k}}$ in terms of $b_{\mathbf{k}}$ and $b^{\dagger}_{-\mathbf{k}}$ in the effective Hamiltonian in Eqn. (3.26), and forcing the coefficient of the off-diagonal terms to be zero we get the following relation:

$$\left[\left[(u_{\mathbf{k}})^2 + (v_{\mathbf{k}})^2\right] Un_0 - 2u_{\mathbf{k}}v_{\mathbf{k}}(e_{\mathbf{k}} + Un_0)\right] = 0 \tag{3.31}$$

Now, we are left with the following effective Hamiltonian,

$$\begin{aligned} H^{eff} &= -\frac{1}{2}Un_0N_0 \\ &+\frac{1}{2}\sum_{\mathbf{k}} \left[(|\, u_{\mathbf{k}} \,|^2 + |\, v_{\mathbf{k}} \,|^2)(e_{\mathbf{k}} + Un_0) - (u^*_{\mathbf{k}}v_{\mathbf{k}} + u_{\mathbf{k}}v^*_{\mathbf{k}})Un_0 - (e_{\mathbf{k}} + Un_0)\right] \\ &+\sum_{\mathbf{k}} \frac{1}{\cancel{2}} \left[\cancel{2}(|\, u_{\mathbf{k}} \,|^2 + |\, v_{\mathbf{k}} \,|^2)(e_{\mathbf{k}} + Un_0) - \cancel{2}(u^*_{\mathbf{k}}v_{\mathbf{k}} + u_{\mathbf{k}}v^*_{\mathbf{k}})Un_0\right] b^{\dagger}_{\mathbf{k}}b_{\mathbf{k}} \end{aligned} \tag{3.32}$$

writing $\left[(|\, u_{\mathbf{k}} \,|^2 + |\, v_{\mathbf{k}} \,|^2)(e_{\mathbf{k}} + Un_0) - (u^*_{\mathbf{k}}v_{\mathbf{k}} + u_{\mathbf{k}}v^*_{\mathbf{k}})Un_0\right]$ as $\hbar\omega$ we can further simplify the above equation as,

$$H^{eff} = -\frac{1}{2}Un_0N_0 + \frac{1}{2}\sum_{\mathbf{k}} \left[\hbar\omega - (e_{\mathbf{k}} + Un_0)\right] + \sum_{\mathbf{k}} \hbar\omega b^{\dagger}_{\mathbf{k}}b_{\mathbf{k}} \tag{3.33}$$

Now, we must find the value of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ by solving the following relations:

$$\begin{aligned} & \left[\left[(u_{\mathbf{k}})^2 + (v_{\mathbf{k}})^2\right] Un_0 - 2u_{\mathbf{k}}v_{\mathbf{k}}(e_{\mathbf{k}} + Un_0)\right] = 0 \text{ and} \\ \hbar\omega &= \left[(|\, u_{\mathbf{k}} \,|^2 + |\, v_{\mathbf{k}} \,|^2)(e_{\mathbf{k}} + Un_0) - (u^*_{\mathbf{k}}v_{\mathbf{k}} + u_{\mathbf{k}}v^*_{\mathbf{k}})Un_0\right] \end{aligned} \tag{3.34}$$

Using the normalization condition $|\, u_{\mathbf{k}} \,|^2 - |\, v_{\mathbf{k}} \,|^2 = 1$ and the above relation we can simplify as,

$$\begin{aligned} \hbar\omega &= \left[(|\, u_{\mathbf{k}} \,|^2 + |\, v_{\mathbf{k}} \,|^2)(e_{\mathbf{k}} + Un_0) - \underbrace{(u^*_{\mathbf{k}}v_{\mathbf{k}} + u_{\mathbf{k}}v^*_{\mathbf{k}})}\, Un_0\right] \\ & \quad \text{by rearranging } (u^*_{\mathbf{k}}v_{\mathbf{k}} + u_{\mathbf{k}}v^*_{\mathbf{k}})\text{as,} \\ &= u_{\mathbf{k}}v_{\mathbf{k}}\frac{(u^*_{k}v_{\mathbf{k}} + u_{\mathbf{k}}v^*_{\mathbf{k}})}{u_{\mathbf{k}}v_{\mathbf{k}}} \\ &= \frac{|\, u_{\mathbf{k}} \,|^2 \, v^2_{\mathbf{k}} - |\, v_{\mathbf{k}} \,|^2 \, u^2_{\mathbf{k}}}{u_{\mathbf{k}}v_{\mathbf{k}}} \end{aligned} \tag{3.35}$$

we have the following terms after rearrangement:

$$\begin{aligned} \hbar\omega &= (1 + 2 \,|\, v_{\mathbf{k}} \,|^2)(e_{\mathbf{k}} + Un_0) - (\frac{|\, u_{\mathbf{k}} \,|^2 \, v^2_{\mathbf{k}} - |\, v_{\mathbf{k}} \,|^2 \, u^2_{\mathbf{k}}}{u_{\mathbf{k}}v_{\mathbf{k}}})Un_0 \\ &= (1 + 2 \,|\, v_{\mathbf{k}} \,|^2)(e_{\mathbf{k}} + Un_0) - (\frac{v_k}{u_k} + \frac{2 \,|\, v_k \,|^2 \, (e_k + Un_0)}{Un_0})Un_0 \end{aligned} \tag{3.36}$$

$$
\begin{aligned}
&= (1+\cancel{2\mid v_{\mathbf{k}}\mid^2})(e_{\mathbf{k}}+Un_0) - (\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} + \cancel{2\mid v_{\mathbf{k}}\mid^2 (e_{\mathbf{k}}+Un_0)})\hbar\omega \\
\hbar\omega &= e_k + Un_0 - \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} \\
\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} &= \frac{e_{\mathbf{k}} + Un_0 - \hbar\omega}{Un_0} \qquad (3.37)
\end{aligned}
$$

using componendo and dividendo with the above relation,

$$
\frac{\frac{v_{\mathbf{k}}+u_{\mathbf{k}}}{\cancel{u_{\mathbf{k}}}}}{\frac{v_{\mathbf{k}}-u_{\mathbf{k}}}{\cancel{u_{\mathbf{k}}}}} = \frac{\frac{e_{\mathbf{k}}+2Un_0-\hbar\omega}{\cancel{Un_0}}}{\frac{e_{\mathbf{k}}-\hbar\omega}{\cancel{Un_0}}} \qquad (3.38)
$$

Now using Eqn. (3.34) and the above relation we get,

$$
\sqrt{1+\frac{2Un_0}{e_{\mathbf{k}}}} = \frac{e_{\mathbf{k}}+2Un_0-\hbar\omega}{e_{\mathbf{k}}-\hbar\omega} \qquad (3.39)
$$

Now taking +1 both sides,

$$
\begin{aligned}
\sqrt{1+\frac{Un_0}{e_k}}+1 &= \frac{2Un_0}{\hbar\omega - e_k} \\
\hbar\omega &= e_k + \frac{2Un_0}{\sqrt{1+\frac{2Un_0}{e_k}}} \qquad (3.40)
\end{aligned}
$$

let $\frac{2Un_0}{e_k} = u$ and simplifying,

$$
\begin{aligned}
\hbar\omega &= e_{\mathbf{k}}\left[1+\frac{u}{\sqrt{1+u}+1}\right] \\
&= e_{\mathbf{k}}\left[1+\frac{\sqrt{1+u}+u+1}{\sqrt{1+u}+1}\right] \\
&= e_{\mathbf{k}}\sqrt{1+u}\left[\cancel{\frac{1+\sqrt{1+u}}{\sqrt{1+u}+1}}\right] \\
&= \hbar\omega = e_{\mathbf{k}}\sqrt{1+u} \\
&= e_{\mathbf{k}}\sqrt{1+\frac{Un_0}{e_{\mathbf{k}}}} \\
\hbar\omega &= \sqrt{e_{\mathbf{k}}^2 + Un_0 e_{\mathbf{k}}} \qquad (3.41)
\end{aligned}
$$

The condensate density n_0 can be obtained by calculating the total density n, given by the effective Hamiltonian as,

$$
n = \frac{1}{N_s}\sum_{\mathbf{k}} \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}\rangle_{H^{eff}} \qquad (3.42)
$$

The density for a condensed Bose gas consists of two parts: the condensates and non condensates. So for the non condensates, their density is due to occupation of the higher lying momentum states.[13][10]. Thus density of non condensate part can be obtained by taking the average of quadratic fluctuations (which should be a function of n_0) and for the condensate density, it can be determined by the parameter n_0. We can calculate the value of this fluctuation using the Eq. (3.42) as,

$$n = n_0 + \frac{1}{N_s}\sum_{\mathbf{k}\neq 0}\left[(\mid u_{\mathbf{k}}\mid^2 + \mid v_{\mathbf{k}}\mid^2)\langle b^\dagger_{\mathbf{k}} b_{\mathbf{k}}\rangle_{H^{eff}} + \mid v_{\mathbf{k}}\mid^2\right] \tag{3.43}$$

using the relations in Eq. (3.41) and substituting the Bose distribution evaluated at $\hbar\omega$ for $\langle b^\dagger_k b_{\mathbf{k}}\rangle_{H^{eff}}$ we get,

$$n = n_0 + \frac{1}{N_s}\sum_{\mathbf{k}\neq 0}\left(\frac{e_{\mathbf{k}} + Un_0}{\hbar\omega_{\mathbf{k}}}\frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1} + \frac{e_{\mathbf{k}} + Un_0 - \hbar\omega_{\mathbf{k}}}{2\hbar\omega_{\mathbf{k}}}\right) \tag{3.44}$$

taking the zero temperature limit i.e. $\beta \longrightarrow \infty$, we have first term zero and now applying the continuum limit $\sum_{\mathbf{k}} \longrightarrow V\int_{-\pi/a}^{\pi/a} d\mathbf{k}/(2\pi)^d$ and changing the momentum from $\mathbf{k}$ to $\mathbf{q}$, $\mathbf{k} = 2\pi a/\mathbf{q}$, we get the following expression,

$$n = n_0 + \frac{1}{2}\int_{-1/2}^{1/2} d\mathbf{q}\left(\frac{e_{\mathbf{k}} + Un_0}{\hbar\omega_{\mathbf{k}}} - 1\right) \tag{3.45}$$

where $e_q = 2t\sum_{j=1}^{d}[1 - cos(2\pi q_i)]$.

for a two dimensional lattice we can calculate the above results numerically [14]. The plot shows condensate fraction n_0/n as a function of energy parameters U/t.

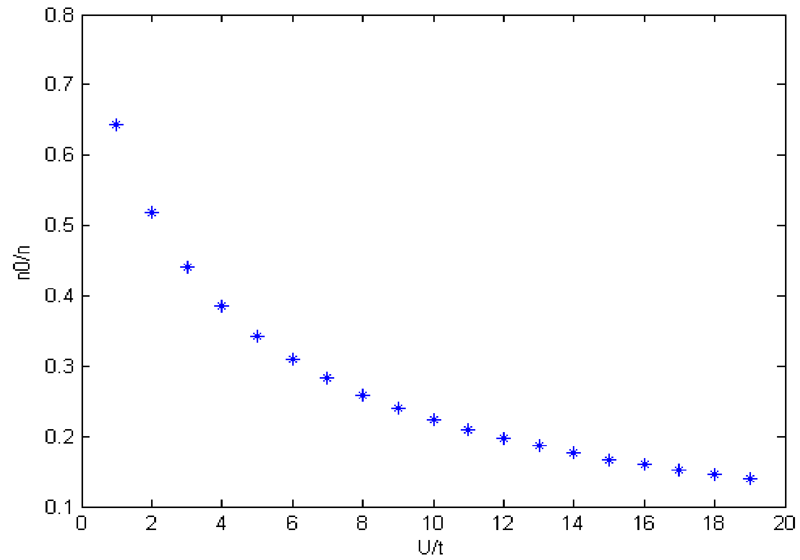

Fig. 3.1: The condensate fraction n_0/n as a function of energy parameters U/t for a one dimensional lattice

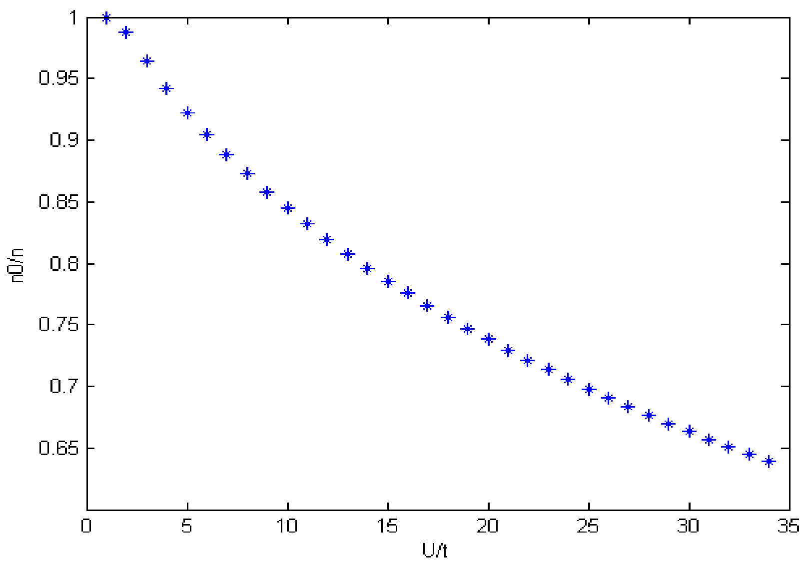

Fig. 3.2: The condensate fraction n_0/n as a function of energy parameters U/t for a two dimensional lattice

4. SUMMARY AND OUTLOOK

In the context of the thesis the theoretical study of experimental signatures of Bose-Einstein Condensates in an optical lattice regime is presented. The idea was to study the formalism and apply it our model where the number of particles is kept constant. First, the Hamiltonian is solved by using HFBP formalism and the condensate density fraction is calculated numerically. The integral involved has a singularity at zero, so it was almost removed by using Gaussian quadrature rule(already implemented in Mathematica). Furthermore, the exchange energy part can be added to the existing Hamiltonian and momentum space density can be calculated to characterize our model. We can also look into the time of flight images for the system and other experimental signatures like visibility(which also depends on the momentum space density) can also be calculated.

5. APPENDIX

5.1 Code for calculation of condensate density fraction n_0/n

In Mathematica and Matlab, I have implemented the eqn. 3.41. The integral involved has a singularity at q=0, so one can basically change the numerical method to get a better picture.

```
Ut = 0;
while Ut<20
f1 = @(n0,x,y)(1+(Ut.*n0)./(2-cos(2.*pi.*x)-

cos(2.*pi.*y))).^-0.5+(1+(Ut.*n0)./(2-cos(2.*pi.*x)
-cos(2.*pi.*y))).^0.5;
a = -0.5;
c = -0.0001;
d = 0.0001;
b = 0.5;
f2 = @(n0)n0+0.5.*(dblquad(@(x,y) f1(x,y,n0),a,c,a,c)

+dblquad(@(x,y) f1(x,y,n0),d,b,d,b))-2;
fig1 = ezplot(f2,0,1);
%n0_guess = [0,1];
%n = fzero(f2,n0_guess);
n = fminbnd(@(n0)abs(f2(n0)),0,1);
fig2 = plot(Ut,n,'*');
hold on
Ut = Ut+1;
end
```

In Mathematica I had better results using its default numerical integration method.

```
Clear[cn, hy, v];

cn[q1_?NumericQ, q2_?NumericQ, n0_?NumericQ,
   Ut_?NumericQ] := ((Ut*n0)/(2 - Cos[2*Pi*q1] - Cos[2*Pi*q2]));
hy[q1_?NumericQ, q2_?NumericQ, n0_?NumericQ, Ut_?NumericQ] :=
  0.25*((1 + cn[q1, q2, n0, Ut])^(-1/2) + (1 + cn[q1, q2, n0, Ut])^(1/
```

```
        2) - 2);
v[n0_?NumericQ, Ut_?NumericQ] :=
  n0 + NIntegrate[
    hy[q1, q2, n0, Ut], {q1, -0.5, 0.5}, {q2, -0.5, 0.5}] - 1;


Clear[n];
n[Ut_?NumericQ] := FindRoot[v[n0, Ut] == 0, {n0, .1}][[1, 2]];
Plot[n[U], {U, 0, 20}, PlotRange -> {{0, 20}, {0, 1}},
 AxesOrigin -> {0, 0},
 AxesLabel -> {"U", "\!\(\*SubscriptBox[\(n\), \(0\)]\)"}]
```

5.2 *Visualization of BECs in optical lattices*

To obtain visualization like Fig. 2.1, we can use eqn. 2.12 to create a periodic potential and then add bosons as per the requirement.

```
r = 25;
p = Show[Plot3D[-Sum[
      4 Exp[-((x - xo)^2 + (y - yo)^2)], {xo, -24, 8, 4}, {yo, -28, 8,
        4}], {x, -r, r - 4}, {y, -r, r - 4}, Evaluated -> True,
    PlotRange -> All, PlotPoints -> 200, Mesh -> 300,
    ImageSize -> 800,
    ColorFunction -> (Blend[{White, White, White, Purple}, -#3] &),
    ColorFunctionScaling -> False,
    MeshStyle -> Directive[Thick, GrayLevel@.4]],
   Graphics3D[{Specularity[White, 15], Green,
     Sphere[{{-3, -3, .2}, {4, 4, .2}, {4, -3, .2}, {-5, -5, .2}, {-5,
         3, .2}, {0, 8, .2}, {4, 3, .2}}, 1]}],
   BoxRatios -> Automatic, Boxed -> False, Axes -> False,
   Lighting -> "Neutral", ViewVector -> {{10, 20, 11}, {0, 0, 0}},
   ViewAngle -> .5];

p = ImageResize[Rasterize[p, "Image", ImageResolution -> 3 72],
  Scaled[1/3]]
```

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